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Widths and intensities of lines in Kβ spectrum of manganese

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Abstract : The widths and intensities of the lines $\beta_{1,3}$, β_5, β' and β''' have been measured on the electron excited and ionometrically recorded Kβ spectrum of manganese.

Keywords Manganese, K spectrum, widths and intensities

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1. Introduction

The Kβ region of X-ray emission spectrum of any element with Z > 10 consists of a strong dipole allowed doublet $K\beta_{1,3}$ $(K-M_{3,2})$ and many weaker lines. In the spectra of elements with Z = 17 to 29, the most intense of these weak lines is the dipole forbidden line $K\beta_5$ $(K-M_{4,5})$. In cases with Z > 29, this line is next in intensity to the dipole allowed line $K\beta_2$ $(K-N_{2,3})$. In these middle and high Z elements, the M shell is a completely filled inner shell of the atom, but in those with Z = 17 to 29, it is the outermost one. In the solids and molecules of these low Z elements the 3d wavefunction is not fully localised to the atom, rather it either takes the form of a molecular orbital (MO) or overlaps with the valence or with the conduction band. Therefore, whereas the $K\beta_5$ line in the spectra with Z > 29 is emitted by a pure electric quadrupole transition $K-M_{4,5}$, in those with Z = 17 to 29, it arises due to a MO transition [1-4], with multipolarity, including the dipole one, to some extent. This makes the line $K\beta_5$ to be more intense than the theoretically calculated ones, assuming it to be a pure quadrupole transition [5-7]. This multipolarity phenomenon has aroused a renewed interest in the measurement of $K\beta_5$ intensity. Torok *et al* [8] have remeasured it in the spectra of $_{20}$Ca, $_{22}$Ti and $_{24}$Cr. These authors have also presented the complete experimental data of $K\beta_5$ intensity in the spectra of elements with Z = 20 to 92, available in literature. It is noted [8] that in the spectra of 3*d* transition elements, with increasing Z, it first increases, becomes maximum at $_{24}$Cr, and then decreases, its values relative to $K\beta_{1,3}$ lines at $_{21}$Sc, $_{24}$Cr and $_{29}$Cu are .015, .04 and .01 respectively. In the range Z > 29, it increases slowly and monotonously, the values at $_{30}$Zn and $_{92}$U being .005 and .03 respectively. The experimental values in the range Z > 29 agree well with Scofield's calculations [5-7].

Besides $K\beta_2$ and $K\beta_5$, other weak lines in K spectra are satellite lines, lying on both high as well as low energy sides of $K\beta_{1,3}$. Amongst the high energy satellites the most intense one is $K\beta'''$, emitted by the $KL_{2,3} - L_{2,3}M_{2,3}$ transitions [9, 10]. This line has been observed in the spectra of almost all the elements with Z = 11 to 47 [11]. The lines on low energy side of $K\beta_{1,3}$ arise mostly due to K – MM radiative Auger transitions [12] and are weaker in intensity than $K\beta'''$. However, in the spectra of 3d transition elements, a stronger line, named $K\beta'$, is observed close to $K\beta_{1,3}$ [13, 14]. This satellite has been assigned to the multiplet splitting of 3p level due to partially filled 3d subshell [13-15]. The intensity of this line relative to $K\beta_{1,3}$ shows a similar variation with Z as that shown by $K\beta_5$, showing a maximum in the middle of 3d series [13, 14]. Though the measured intensities are lower than the theoretically calculated ones, the variation with Z agrees with theory [13-15].

Looking to the behaviour of $K\beta_5$ and $K\beta'$ intensities due to the involvement of 3d orbitals in their emission, the precisely measured intensities of these lines in $K\beta$ spectra of 3d transition metals are more helpful in understanding the models proposed [5-7, 13-15] for their emission. In the present paper, I report the results of such measurements in the $K\beta$ spectrum of metallic manganese. Earlier measured values, available in literature are also presented for comparison.

2. Experiment

The K-emission spectrum of manganese was excited in a demountable tube by a 10 keV – 1.5 mA beam of electrons emitted from a V shaped hot tungsten filament. The anode was fine metallic powder of manganese, of 99.9% purity and known impurities, and was pressed gently on the roughened surface of an aluminium anticathode. The tube was operated at a vacuum of nearly 10^{-4} Pa. The spectra were analysed by a plane crystal spectrometer operated with a stepper motor. A Topaz crystal ($2d$ = 2.712 Å) was used as the analyser, which was rotated in steps of 0.01°. The horizontal divergences of incoming and outgoing beams were limited to 0.15° and 0.40° with the help of Soller slits provided on the spectrograph arms. The detector was a proportional counter in which a mixture of 90% argon and 10% methane was flowing continuously. The counter was associated with necessary electronics leading to a teletype printer on which accumulated counts at each step of the crystal position were recorded on a punch tape as well as on a digital printer. The spectra were scanned several times, collecting number of counts at each step for a known time interval. The sum of three such scans is shown in Figure 1.

3. Measurements and results

The $K\beta$ spectrum of manganese (Figure 1) consists of two asymmetric line like structures, marked "A" and "B" corresponding to $K\beta_{1,3}$ and $K\beta_5$ respectively. The B part has been plotted on magnified scale also. The curve A has a pronounced shoulder on its low energy tail, due to the satellite $K\beta'$ while B has an extended high energy tail due to $K\beta'''$. Each of these curves has been resolved geometrically into two components as follows.

The background for the curve A has been taken as a straight line, drawn below it, in Figure 1. Assuming that low energy tail below half maximum of $K\beta'$ and high energy tail below half maximum of $K\beta_{1,3}$ are not affected significantly by the contribution of the other line in this A peak, and assuming that each of $K\beta_{1,3}$ and $K\beta'$ is a symmetric line, the two resolved parts have been obtained graphically by trial and error method. In these trials, the separation between two peaks has been kept fixed, the 12.28 eV [11], and the heights and widths have been varied till the envelope agrees well with the measured curve A.

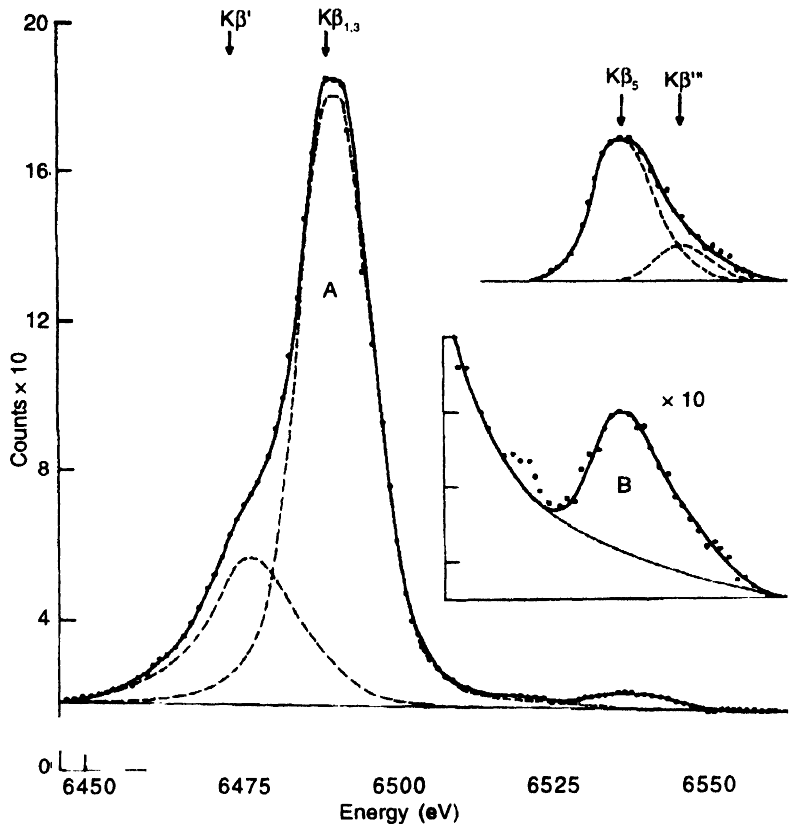

Figure 1. The $K\beta_{1,3}$ and $K\beta_5$ spectrum of manganese The $K\beta_5$ part has been plotted on magnified scale also The straight line below the peak A is the assumed background of the $K\beta_{1,3}$ spectrum while the curve below B is the Lorentzian tail part of $K\beta_{1,3}$ peak and assumed as the background for this peak B The curve above B is the pure $K\beta_5$ spectrum obtained after subtracting this background from the measured curve B. For resolution of each of the peaks A and B into two component lines see text. The resolved parts are shown by dashed curves and their envelope by the bold continuous curves.

For the structure B, the background has been taken as the tail part of $K\beta_{1,3}$ line calculated by assuming it to be a Lorentzian curve. This background has been shown in the enlarged version of peak B in Figure 1. Above this peak, in the inset, the structure calculated by subtracting this background curve from the measured curve B has been shown. This curve has then been resolved into two curves graphically in the same manner as that adopted for peak A above. However in doing so, the separation between $K\beta_5$ and Kβ''' has also been found necessary to be adjusted slightly, from 7.0 eV [11] to 9.4 eV. The two resolved parts have been shown in the envelope in the inset.

The measurements of widths and peak heights as well as areas under the curve representing each line have been done on these so calculated curves and are given in Table 1. The values measured by earlier researchers are also given for comparison. It is noted that our values for Kβ' and Kβ'''agree well with the earlier measured values [14, 16]. For $K\beta_5$ intensity, Torok *et al* [8] have presented the earlier measured values as 1.45, 1.83 and 2.83 % relative to $K\beta_{1,3}$. Their own graphical estimation of this intensity from one of the earlier reported spectra is 2.16%. This value is in excellent agreement with the sum of $K\beta_5$ and Kβ' intensities measured presently.

Table 1. Widths and intensities of Kβ lines of Manganese.

Line	FWHM (eV)	Intensity (a)	
		Peak height	Area
$K\beta_{1,3}$	10.94	100	100
$K\beta_5$	10 60	2.470 ± 0.085	1.843 ± 01 1 45 to 2 83 [8]
Kβ'	16.47	32 5 ± 0.9	29.8 ± 1 5 30.2 ± 3 0 [14]
Kβ'''	9 82	0 653 ± 0 01	0 353 ± 0 01 0.357 [16]

(a) All intensities are relative to that of $K\beta_{1,3}$ line which has been arbitrarily taken as 100 Earlier reported values are given below the present ones. The earlier value for $K\beta_5$ has been estimated from Figure 4 of Ref. [8]

4. Conclusion

It has been established that the $K\beta_5$ intensity in the spectrum of manganese is higher than the theoretical value expected by assuming it to be a pure electric quadrupole line. The only experimental measurement of Kβ' intensity by Salem *et al* [14] has been confirmed, thereby suggesting that the simple theoretical model presented by these authors [14] for its intensity need a thorough theoretical reinvestigation.

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